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A QUALITATIVE STUDY OF THE STEADY-STATE SOLUTIONS FOR A CONTINUOUS FLOW STIRRED TANK CHEMICAL REACTOR*

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Abstract. An approach to the bifurcation of steady-state equilibria using singularity theory is applied to the problem of multiple equilibria in a continuous flow stirred tank chemical reactor where the flow rate is the bifurcation parameter. Under the assumption of a single first-order exothermic chemical reaction, all the qualitatively different bifurcation diagrams which occur locally are found. They form the universal unfolding of the singular bifurcation problem $x^3+\lambda^2=0$.

Introduction. It is well-known to chemical engineers that a complex reacting system can exhibit multiple equilibria which may differ dramatically from each other as to the extent of the reaction, the equilibrium temperature, and other phenomena. Analysis of this sort of problem is complicated by the fact that the equations are highly nonlinear, and contain many parameters, or control variables, which affect the configuration of the equilibria. This paper is an attempt to bring a new method to bear on such problems by the application of singularity theory to a chemical reactor problem. Singularity theory is a nonlinear theory which provides a framework for a qualitative analysis of many-parameter problems via the notions of contact equivalence, in terms of which "qualitatively similar" behavior can be precisely defined, and a universal unfolding, by means of which essential parameters can be identified. When a particular universal unfolding can be found for a complex problem, it may then be regarded as a perturbation of a simpler problem with the parameters varied about a particular choice. We feel that this technique, of building up a complete description of the solution from the behavior near this particular choice, or "organizing center" of the problem, may be widely applicable in those chemical engineering and combustion problems where a diversity of multiple steady-state phenomena makes any global analysis very difficult. The possibility of providing such a description was suggested by some work of Uppal, Ray and Poore [6], [7], on a continuous flow stirred tank reactor model in which an analysis of the steady-state behavior is a prerequisite for an understanding of the dynamic behavior of the model. Uppal, Ray and Poore were unable to prove that their analysis was complete, but provided some partial results supplemented by numerical experiments. Using singularity theory, we have been able to show that they did indeed identify all the qualitatively different types of equilibrium behavior of the system, and that the same classification also applies to a generalized system in which the standard temperature dependence of the reaction is replaced by a function with similar properties. To be precise, Uppal, Ray and Poore consider a single-step chemical reaction with Arrhenius-type kinetics, that is a reaction rate term of the form $\exp(-E/RT)$. For a class of reaction rate terms which includes a C^3-open neighborhood of the Arrhenius terms, we show that the structure of solutions is the same. In § 1, we describe the model used by Uppal, Ray and Poore and its generalization.

For physical reasons it is often convenient to analyze the steady states of a system by examining the dependence of these states on a distinguished parameter which is

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varied "quasi-statically"—i.e., the system is supposed always to remain in equilibrium. Of particular interest are the parameter values where the number of equilibria changes (bifurcation of equilibria)—hence the term "bifurcation parameter" which will be used to describe this variable throughout the paper. Although the approach to the reactor and similar systems as bifurcation problems is natural, classical bifurcation theory (for example [3]) has generally not considered such problems because there is no "trivial solution" about which to look for bifurcation points. Instead, we have the familiar S-curves of combustion theory. The recent approach of Golubitsky and Schaeffer [4] to bifurcation problems via singularity theory extends and specializes the theorems and techniques of singularity theory to steady-state bifurcation problems, and it is this theory that we apply to the reactor problem. Specifically the theorems of singularity theory are adapted to include the bifurcation parameter indicated above as a distinguished control variable. A brief description of the theory and an analysis of the singularities that appear in this problem are given in § 2. The "organizing center" for the problem turns out to be a singularity we have named the *winged cusp*: it corresponds to a particular, physically reasonable, choice of control variables. This singularity is of codimension three: that is, three independent controls must be varied in the neighborhood of the organizing center to yield all the qualitatively different types of bifurcation diagrams. These perturbed bifurcation diagrams are also listed in § 2. In § 3 we verify that the winged cusp singularity is present in this problem, and that the physical parameters do indeed provide a complete set of perturbations (or "unfolding parameters") not only near the organizing center but everywhere in control space.

We are grateful to Rutherford Aris for pointing out this problem to us, and would like to thank David Schaeffer for many helpful conversations. Articles by Ray [5] and Aris [1], where an attempt was made to adapt the catastrophe theory cusp, by the addition of a wing, to explain the results of Uppal, Ray and Poore, served as a guide for our intuition. Elementary catastrophe theory now seems an inappropriate theory for the analysis of this model, although the type of mathematics ultimately used is identical in spirit to that of elementary catastrophe theory. Needless to say, our name for the organizing center of this problem, the winged cusp, was motivated by the papers of Ray and Aris.

1. A mathematical model for a continuous flow stirred tank chemical reactor. In this section we derive an equation to describe the steady-state temperature and concentration for a first-order, single-step, exothermic, irreversible, volume-preserving chemical reaction which takes place in a continuously stirred tank with in- and out-flow, and heat loss to the surroundings. If a reactant, $\mathscr{R}$, is converted to a product, $\mathscr{P}$, in the reaction, the assumption that the tank is stirred permits the concentration of $\mathscr{R}$, c, and the temperature inside the tank, T, to be described as functions of time, t', alone, while the heat-loss rate is modeled by a term of the form $-hS(T-T_0)$, where T_0 is the ambient temperature and h is a heat-transfer coefficient which depends on the thermal conductivity of the mixture and of the walls, and S is the heat-transfer area (surface area of the container). In the reaction, $\mathscr{R}$ is converted to $\mathscr{P}$ at a rate $k(T)c$, where $k(T)$ is the temperature-dependent reaction rate. For chemical reactor problems, in which radiation is usually ignored, $k(T)$ is assumed to have a temperature dependence of the Arrhenius form,

$$k(T)=Z\,e^{-(E/RT)}, \tag{1.1}$$

where Z is a frequency factor and E is called the *activation energy* of the reaction. The constant R is the Boltzmann constant. The heat release of such a reaction is $(-\Delta H)k(T)$, where ΔH, the heat of reaction, is negative for an exothermic reaction.

Finally, if reactant with concentration c_f and temperature T_f are fed into the tank at a flow rate F, and the mixture of reactant and product removed at the same rate, the equations governing the time-evolution of T and c are

$$\begin{aligned} V\frac{dc}{dt'} &= F(c_f-c) - Vk(T)c, \\ V\rho C_\rho \frac{dT}{dt'} &= \rho C_\rho F(T_f - T) + V(-\Delta H)k(T)c - hS(T-T_0), \end{aligned} \tag{1.2}$$

where V is the volume of the container and ρ and C_ρ are the density and specific heat of the mixture (assumed constant). This standard system is discussed in [6], [1].

The following scalings are also conventionally used to develop nondimensionalized equations. Concentration and temperature are scaled by feeder concentration and temperature so that

$$x = \frac{c_f - c}{c_f} \tag{1.3}$$

measures the extent of conversion of $\mathscr{R}$ to $\mathscr{P}$, and

$$y = \frac{T - T_f}{T_f} \tag{1.4}$$

is the rise above entrance temperature. Note that $y > -1$. Time is conveniently scaled by the heat-transfer rate,

$$t = \frac{hS}{V\rho C_\rho} t'. \tag{1.5}$$

Then (1.2) is replaced by

$$\begin{aligned} \frac{dx}{dt} &= -\varepsilon x + D(1-x)A(y) = f_1(x, y), \\ \frac{dy}{dt} &= -(1+\varepsilon)y + BD(1-x)A(y) + \eta = f_2(x, y), \end{aligned} \tag{1.6}$$

where now the essential parameters appearing are

$$\varepsilon = \frac{F\rho C_\rho}{hS} = \frac{1}{\theta}, \tag{1.7}$$

which can be identified as a flow-rate based on the time-scale (1.5) (its reciprocal, θ, is called the *residence time*, and is often in the literature taken as the fundamental flow-rate parameter),

$$D = \frac{k(T_f)V\rho C_\rho}{hS}, \tag{1.8}$$

a Damköhler number relating the chemical heat-gain rate at T_f to the heat-loss rate,

$$B = \frac{(-\Delta H)C_f}{\rho C_\rho T_f}, \tag{1.9}$$

which is proportional to the exothermicity, and also measures the "adiabatic temperature rise" which would occur if the reaction proceeded to completion in the absence of heat-loss or flow in the reactor, and

$$\eta = \frac{T_0 - T_f}{T_f}, \tag{1.10}$$

the ambient temperature scaled by (1.4).

The function

$$A(y) = \frac{k(T_f y + T_f)}{k(T_f)} \tag{1.11}$$

is the temperature-dependent reaction rate, scaled by the rate at T_f. For an Arrhenius temperature dependence,

$$A(y) = \exp\left(\frac{\gamma y}{1+y}\right), \tag{1.12}$$

where

$$\gamma = \frac{E}{RT_f} \tag{1.13}$$

is a scaled activation energy. For a truly temperature-dependent reaction, γ cannot be too small, and, in fact, in many applications to ignition problems, y is further scaled by $\bar{y} = \gamma y$ and the approximation $\gamma = \infty$ is used. Alternatively, $A(y)$ is often approximated by a low-degree polynomial for the range of y known to occur in some particular problem. These approximations are introduced to make computations simpler, and will, in general, change the qualitative properties of solutions of (1.6) outside the range in which they are valid. In the present paper, we will not insist that $A(y)$ be an Arrhenius term, but we will, in § 3, impose on $A(y)$ a set of conditions, satisfied by all Arrhenius terms with $\gamma > 8/3$, which will guarantee a certain qualitative behavior for steady-state solutions of (1.6).

The system (1.6) has the property that multiple steady states, that is solutions to $f_1 = f_2 = 0$, can exist for certain values of the parameters ε, D, B and η. In this paper, we shall classify these steady states by means of the bifurcation diagrams which occur when D, B and η are regarded as fixed control parameters, and ε is varied quasi-statically as a bifurcation parameter. This was the approach of Uppal, Ray and Poore in [7]. While it is possible to regard any of the parameters as a bifurcation variable, in any experiment it is clear that ε can be varied independently by adjusting the flow rate, while it would be difficult to design an experiment in which changing a single physical variable changed only one other dimensionless variable.

Thus, in what follows, a "bifurcation diagram" is defined as the graph of the steady-state solutions of (1.6) versus ε. The description is simplified somewhat in this problem because x or y can be eliminated from the equations $f_1 = f_2 = 0$ and the equilibrium is determined by a single state variable, temperature or concentration, alone. Since (1.6) is linear in x, it is convenient to eliminate x by

$$x = \frac{DA(y)}{\varepsilon + DA(y)} = \frac{\eta - (1+\varepsilon)y + BDA(y)}{BDA(y)}. \tag{1.14}$$

Introducing the notation $\delta = 1/D$ and $\mathcal{A}(y) = 1/(A(y))$, we find the equilibrium temperature satisfies $G = 0$, where

$$G(y, \varepsilon, B, \delta, \eta) = \eta - (1+\varepsilon)y + \frac{B\varepsilon}{1 + \varepsilon\delta\mathcal{A}(y)}. \tag{1.15}$$

All the qualitative analysis of the bifurcation diagrams is based on an analysis of the C^∞ function G.

2. The theory. In this section we shall state the theorems of [4] specialized to one state variable and discuss in detail the "winged cusp" singularity which we claim is the organizing center for the bifurcation problem associated to the stirred tank reactor described in § 1.

Let $\mathscr{E}_{x,\lambda}$ be the space of C^∞ germs of mappings from $\mathbb{R}^2 \to \mathbb{R}$ at 0 depending on the variables x and λ. A *bifurcation problem* is the solution of

$$G(x, \lambda) = 0, \tag{2.1}$$

where $G(0, 0) = 0$ for G in $\mathscr{E}_{x,\lambda}$. Two bifurcation problems G and H are *contact equivalent* if

$$G(x, \lambda) = T(x, \lambda)H(X(x, \lambda), \Lambda(\lambda)), \tag{2.2}$$

where $T(0, 0) \neq 0$, $(\partial X/\partial x)(0) > 0$, $(\partial\Lambda/\partial\lambda)(0) > 0$, and $X(0) = \Lambda(0) = 0$. We shall use contact equivalence as our formalization of the term "qualitatively similar" for bifurcation problems as discussed in the Introduction.

There are two problems about contact equivalence which need to be investigated in order to analyze the stirred tank reactor. Although these problems have similar statements their resolution requires different methods. First, when is a bifurcation problem G contact equivalent to a (simple) polynomial and if it is how does one find this normal form? Second, we ask this question for a k-parameter family of given bifurcation problems. As we shall see the theoretical answer to both questions is the same although the mathematical sophistication needed to prove the second is of a much higher order.

Let

$$\tilde{T}G = \left\langle G, \frac{\partial G}{\partial x} \right\rangle \tag{2.3}$$

be the ideal in $\mathscr{E}_{x,\lambda}$ generated by G and $\partial G/\partial x$; that is, all function germs of the form

$$a(x, \lambda)G(x, \lambda) + b(x, \lambda)\frac{\partial G}{\partial x}(x, \lambda),$$

where $a, b \in \mathscr{E}_{x,\lambda}$.

DEFINITION 2.4. G has *finite codimension* if there exists a finite dimensional vector space $V \subset \mathscr{E}_{x,\lambda}$ such that $\tilde{T}G \oplus V = \mathscr{E}_{x,\lambda}$.

Theorem 2.8 of [4] states that if G has finite codimension then G is contact equivalent to a polynomial. More interesting is the question of how one finds this normal form. The main step is given by the following proposition whose proof is elementary, requiring only the standard existence theorem for ordinary differential equations, and is a special case of the discussion after Lemma 3.8 of [4].

PROPOSITION 2.5. *Let $H = G + P$ and define G_t to be $G + tP$. Then H is contact equivalent to G if $\tilde{T}G_t = \tilde{T}G$ for $0 \leqq t \leqq 1$.*

The following is useful for checking the hypothesis of Proposition 2.5. Let $\mathscr{M} = \langle x, \lambda \rangle$ be the maximal ideal generated by x and λ.

LEMMA 2.6 (Nakayama's lemma). *Let $\mathscr{I} = \langle p_1, \cdots, p_k \rangle$ be the ideal in $\mathscr{E}_{x,\lambda}$ generated by $p_1, \cdots, p_k$ and suppose that $q_1, \cdots, q_k$ are in $\mathscr{M}\mathscr{I}$. Then $\mathscr{I} = \langle p_1 + q_1, \cdots, p_k + q_k \rangle$.*

Note. $\mathcal{M}\mathcal{I}$ denotes the product of the ideals $\mathcal{M}$ and $\mathcal{I}$ and is the ideal generated by the products of the generators of $\mathcal{M}$ and $\mathcal{I}$.

Proof. See, for example, Lemma 3.10 of [4].

Before discussing the second problem we analyze two bifurcation problems which both occur in the stirred tank problem and serve as examples of the general theory.

PROPOSITION 2.7. *Let $H(x, \lambda)$ satisfy one of the following set of conditions:*

$$\bar{H} = \bar{H}_x = \bar{H}_\lambda = \bar{H}_{xx} = \bar{H}_{x\lambda} = 0 \quad \text{and} \quad \bar{H}_{xxx}\bar{H}_{\lambda\lambda} > 0, \tag{2.8a}$$

$$\bar{H} = \bar{H}_x = \bar{H}_\lambda = \det\,(\overline{d^2H}) = 0 \quad \text{and} \quad \bar{H}_{xx}\overline{d^3H}(v, v, v) > 0, \tag{2.8b}$$

where the bar indicates evaluation at $x = \lambda = 0$ and $v \neq 0$ satisfies $(\overline{d^2H})(v) = 0$. Then (i) *$\tilde{T}H$ is computed to be*

$$\langle \lambda^2, x^2 + 2(\bar{H}_{xx\lambda}/\bar{H}_{xxx})x\lambda \rangle \tag{2.9a}$$

or

$$\left\langle \lambda^3, x + \frac{\bar{H}_{x\lambda}}{\bar{H}_{xx}}\lambda + \left(\frac{\bar{H}_{x\lambda\lambda}}{2\bar{H}_{xx}} - \frac{\bar{H}_{x\lambda}\bar{H}_{xx\lambda}}{\bar{H}_{xx}^2} + \frac{\bar{H}_{x\lambda}^2\bar{H}_{xxx}}{2\bar{H}_{xx}^3}\right)\lambda^2 \right\rangle \tag{2.9b}$$

and (ii) *H is contact equivalent to*

$$x^3 + \lambda^2 \tag{2.10a}$$

or

$$x^2 + \lambda^3 \tag{2.10b}$$

respectively.

Note. We call the bifurcation problem $G(x, \lambda) = x^3 + \lambda^2$ a *winged cusp.*

Proof. The main part of the proof is the computation of $\tilde{T}H$. We show first how (ii) follows from this computation along with Proposition 2.5. The assumption (2.8a) implies

$$H(x, \lambda) = a\lambda^2 + bx^3 + cx^2\lambda + dx\lambda^2 + e\lambda^3 + Q(x, \lambda), \tag{2.11a}$$

where $Q(x, \lambda)$ begins with terms of order four and $ab > 0$. Observe that by a change in coordinates of the form $x = \tilde{x} + B\lambda$ we can assume that $2c = \bar{H}_{xx\lambda} = 0$. After this preliminary change of coordinates the computation of $\tilde{T}H$ given by (2.9a) shows that $\tilde{T}H = \langle \lambda^2, x^2 \rangle$. Let $P = dx\lambda^2 + e\lambda^3 + Q(x, \lambda)$ and apply Proposition 2.5 to see that H is contact equivalent to $bx^3 + a\lambda^2$. Since multiplication by -1 and scaling are contact equivalences (2.10a) is proved. As case (b) of Proposition 2.7 is similar we just point out briefly that assumption (2.8b) implies

$$H(x, \lambda) = ax^2 + bx\lambda + c\lambda^2 + dx^3 + ex^2\lambda + fx\lambda^2 + g\lambda^3 + Q(x, \lambda), \tag{2.11b}$$

where Q is as above and $a \neq 0$. The computation of $\tilde{T}H$ given in (2.9b) shows that if we can make preliminary changes of coordinates so that $b = f = 0$ then (2.10b) will follow from Proposition 2.5. The assumption that $\det\,(\overline{d^2H}) = 0$ implies

$$ax^2 + bx\lambda + c\lambda^2 = a\left(x + \frac{b}{2a}\lambda\right)^2. \tag{2.12}$$

Letting $\tilde{x} = x + (b/2a)\lambda$ puts H in the form (2.11b) with $b = c = 0$. A short calculation shows that letting $\tilde{x} = \tilde{\tilde{x}} + B\lambda^2$ will now put H in the form (2.11b) with $f = 0$ also.

To compute (2.9a) and (2.9b) we will make repeated use of Nakayama's lemma along with the following simple observation. Let P, A, B, f be in $\mathscr{E}_{x,\lambda}$. Then

$$\langle A, P\rangle = \langle B, P\rangle \quad \text{if } A = B + fP. \tag{2.13}$$

First we compute (2.9a). From (2.11a) we see that

$$\tilde{T}H = \left\langle \lambda^2 + C, x^2 + \frac{2c}{3b} x\lambda + C' \right\rangle, \tag{2.14}$$

where C and C' begin with terms of order three. Observe that

$$\mathscr{M}^3 \subset \mathscr{M}\left\langle \lambda^2, x^2 + \frac{2c}{3b} x\lambda \right\rangle$$

so that Nakayama's lemma implies

$$\tilde{T}H = \left\langle \lambda^2, x^2 + \frac{2c}{3b} x\lambda \right\rangle. \tag{2.15}$$

As $c = \bar{H}_{xx\lambda}/2$ and $b = \bar{H}_{xxx}/6$ (2.9a) is proved.

To compute (2.9b) observe that (2.11b), (2.12), and (2.13) imply

$$\tilde{T}H = \langle dx^3 + ex^2\lambda + fx\lambda^2 + g\lambda^3 + Q', 2ax + b\lambda + 3dx^2 + 2ex\lambda + f\lambda^2 + C\rangle, \tag{2.16}$$

where $C = \text{cubic} + \cdots$ and $Q' = \text{quartic} + \cdots$. Note that $x + (b/2a)\lambda \equiv \text{quadratic} + \cdots \bmod \tilde{T}H$; thus $(x + (b/2a)\lambda)^2 \equiv \text{quartic} + \cdots \bmod \tilde{T}H$. Hence the cubic terms in the first generator of $\tilde{T}H$ in (2.16) are the same as the cubic terms of H as in (2.11b). Next observe that $x \equiv -(b/2a)\lambda + \cdots \bmod \tilde{T}H$; thus (2.16) implies

$$\tilde{T}H = \langle K\lambda^3 + Q''(\tilde{x}, \lambda), \tilde{x} + C'(\tilde{x}, \lambda)\rangle, \tag{2.17}$$

where $K = \overline{(d^3H)}(v, v, v) \neq 0$ and $\tilde{x} = 2ax + b\lambda + 2ex\lambda + 3dx^2 + f\lambda^2$. To see that K is as claimed one needs the following observation:

$$6(d^3\bar{H})(v, v, v) = -\bar{H}_{xxx}\left(\frac{\bar{H}_{x\lambda}}{\bar{H}_{xx}}\right)^3 + 3\bar{H}_{xx\lambda}\left(\frac{\bar{H}_{x\lambda}}{\bar{H}_{xx}}\right)^2 - 3\bar{H}_{x\lambda\lambda}\left(\frac{\bar{H}_{x\lambda}}{\bar{H}_{xx}}\right) + \bar{H}_{\lambda\lambda\lambda}, \tag{2.18}$$

which is obtained from the fact that v may be taken to be $(-\bar{H}_{x\lambda}/\bar{H}_{xx}, 1)$.

Since $a \neq 0$, $\tilde{x}$ is a legitimate change of coordinates. One may use Nakayama's lemma in the $\tilde{x}$, λ coordinates to obtain

$$\tilde{T}H = \langle \lambda^3, \tilde{x}\rangle = \left\langle \lambda^3, x + \frac{b\lambda + f\lambda^2}{2a + 3dx + 2e\lambda} \right\rangle \tag{2.19}$$

so $\mathscr{M}^3 \subset \tilde{T}H$. Next compute

$$\frac{b\lambda + f\lambda^2}{2a + 3dx + 2e\lambda} \equiv \frac{b}{2a}\lambda + \left(\frac{f}{2a} - \frac{be}{2a^2}\right)\lambda^2 - \frac{3bd}{4a^2} x\lambda \quad (\text{mod } \mathscr{M}^3). \tag{2.20}$$

Therefore using (2.13) we have

$$\tilde{T}H = \left\langle \lambda^3, x + \frac{b}{2a}\lambda + \left(\frac{f}{2a} - \frac{be}{2a^2} + \frac{3b^2d}{8a^3}\right)\lambda^2 \right\rangle. \tag{2.21}$$

Using the fact that $a = \bar{H}_{xx}/2$, $b = \bar{H}_{x\lambda}$, $d = \bar{H}_{xxx}/6$, $e = \bar{H}_{xx\lambda}/2$, and $f = \bar{H}_{x\lambda\lambda}/2$ the proposition is proved.

We now turn to the second problem; polynomial normal forms for k-parameter families of bifurcation problems. This is formalized through the notion of unfoldings and solved through the notion of universal unfoldings.

DEFINITION 2.22. (i) F: $(\mathbb{R}\times\mathbb{R}\times\mathbb{R}^k, 0)\to\mathbb{R}$ is a *k-parameter unfolding* of G in $\mathscr{E}_{x,\lambda}$ if $F(x,\lambda,0)=G(x,\lambda)$.

(ii) Let $H(x,\lambda,\beta)$ be an m-parameter unfolding of G. Then *H factors through F* if

$$H(x,\lambda,\beta)=F(X(x,\lambda,\beta),\Lambda(\lambda,\beta),\alpha(\beta)), \tag{2.23}$$

where all mappings are smooth and $\alpha(0)=0$.

(iii) Two unfoldings H and F are *equivalent* if H factors through F and the map $\alpha\to\beta(\alpha)$ in (2.23) is an invertible change in coordinates (so $m=l$).

(iv) F is a *universal unfolding*[1] of G if every unfolding H factors through F.

Note (a). The number of parameters in H need not be the same as the number in F.

Note (b). Equation (2.23) means that for every β, $H(\cdot,\cdot,\beta)$ is contact equivalent to $F(\cdot,\cdot,\alpha)$ for some α. Thus, if H factors through F then every bifurcation problem included in the unfolding H is already included in the unfolding F, at least up to contact equivalence.

In what follows we shall show why it is relatively easy to put a universal unfolding into a polynomial normal form.

PROPOSITION 2.24. *Let F and H be universal unfoldings of G depending on the same number of parameters. Then F and H are equivalent.*

Proof. Proposition 2.5 of [4].

THEOREM 2.25. *Let $F(x,\lambda,\alpha)$ be an l-parameter unfolding of $G(x,\lambda)$ and assume that G has finite codimension. Then F is a universal unfolding if*

$$\mathscr{E}_{x,\lambda}=\tilde{T}G+\mathscr{E}_\lambda\left\{\frac{\partial G}{\partial\lambda}\right\}+\mathbb{R}\left\{\left.\frac{\partial F}{\partial\alpha_1}\right|_{\alpha=0},\cdots,\left.\frac{\partial F}{\partial\alpha_k}\right|_{\alpha=0}\right\}. \tag{2.26}$$

Proof. Theorem 2.4 of [4].

We see from (2.26) that G has a universal unfolding precisely when G has finite codimension. The following remarks should make this clear.

Note. Equation (2.26) may be restated as follows: for every germ $p(x,\lambda)$ there exist function germs $a(x,\lambda)$, $b(x,\lambda)$, and $c(\lambda)$—*not* $c(x,\lambda)$—and real numbers $r_1,\cdots,r_k$ such that

$$p(x,\lambda)=a(x,\lambda)G+g(x,\lambda)\frac{\partial G}{\partial x}+c(\lambda)\frac{\partial G}{\partial\lambda}+r_1\frac{\partial F}{\partial\alpha_1}(x,\lambda,0)+\cdots+r_k\frac{\partial F}{\partial\alpha_k}(x,\lambda,0). \tag{2.27}$$

This condition may look difficult to check but, in reality, it is not. Consider:

Example 2.28. Let $G(x,\lambda)=x^3+\lambda^2$. Then $F(x,\lambda,\alpha_1,\alpha_2,\alpha_3)=x^3+(\alpha_2\lambda+\alpha_3)x+\alpha_1+\lambda^2$ is a universal unfolding of G. Moreover codim $G=3$.

DEFINITION 2.29. The *codimension* of G is the minimum number of parameters necessary for a universal unfolding of G.

Proof. From (2.9a), $\tilde{T}G=\langle x^2,\lambda^2\rangle$. Hence (2.27) becomes

$$p(x,\lambda)=a(x,\lambda)x^2+b(x,\lambda)\lambda^2+c(\lambda)\lambda+r_1+r_2\lambda x+r_3x. \tag{2.30}$$

It is easy to check that (2.30) holds for all p by Taylor's theorem.

[1] In the literature the term "universal" is reserved for the unfolding in (iv) with the minimum number of parameters, and "versal" for what we have defined. We shall not make this distinction.

All of the germs G that will be considered in this paper have the property that $\lambda(\partial G/\partial\lambda)$ is contained in $\tilde{T}G$. As a result (2.26) may be reduced to a question of linear algebra.

COROLLARY 2.31. *Assume $\lambda(\partial G/\partial\lambda)$ is in $\tilde{T}G$, and let $q_1(x,\lambda),\cdots,q_s(x,\lambda)$ be a basis for a complementary subspace to $\tilde{T}G$ in $\mathscr{E}_{x,\lambda}$. Let $F(x,\lambda,\alpha)$ be an l-parameter unfolding of $G(x,\lambda)$.*
Let

$$\frac{\partial F}{\partial \alpha_i}(x,\lambda,0)=c_{i,1}q_1+\cdots+c_{i,s}q_s+t_i$$

and

$$\frac{\partial G}{\partial \lambda}(x,\lambda)=c_{l+1,1}q_1+\cdots+c_{l+1,s}q_s+t_{l+1},$$

where t_i is in $\tilde{T}G$ for $1\leqq i\leqq l+1$. Then F is a universal unfolding if rank $C=s$ *where $C=(c_{ij})$ is the $(l+1)\times s$ matrix described above.*

Note. Example 2.28 is now a triviality as a complementary space to $\langle x^2,\lambda^2\rangle=\tilde{T}G$ is spanned by $1, x, \lambda, x\lambda$.

Examples of the application of Theorem 2.25 and its Corollary 2.31 in identifying universal unfoldings can be found in [4]. We provide the specific results for the new singularities—the winged cusp $(x^3+\lambda^2)$ and $x^2+\lambda^3$—which arise in the present application in the next proposition.

PROPOSITION 2.32. *Let $F(x,\lambda,\alpha_1,\alpha_2,\alpha_3)$ be an unfolding of $G(x,\lambda)$. Assume that* (i) *G satisfies* (2.8a) *and suppose that* rank $C=4$ *where C is the matrix*

$$\begin{pmatrix} F_{\alpha_1} & F_{\alpha_1 x} & F_{\alpha_1\lambda} & F_{\alpha_1 x\lambda}-\dfrac{G_{xx\lambda}}{G_{xxx}}F_{\alpha_1 xx} \\ F_{\alpha_2} & F_{\alpha_2 x} & F_{\alpha_2\lambda} & F_{\alpha_2 x\lambda}-\dfrac{G_{xx\lambda}}{G_{xxx}}F_{\alpha_2 xx} \\ F_{\alpha_3} & F_{\alpha_3 x} & F_{\alpha_3\lambda} & F_{\alpha_3 x\lambda}-\dfrac{G_{xx\lambda}}{G_{xxx}}F_{\alpha_3 xx} \\ 0 & 0 & G_{\lambda\lambda} & G_{x\lambda\lambda}-\dfrac{G_{xx\lambda}^2}{G_{xxx}} \end{pmatrix}$$

evaluated at $x=\lambda=0$, or

(ii) *G satisfies* (2.8b) *and suppose that* rank $C=2$ *where C is the matrix*

$$\begin{pmatrix} F_{\alpha_1} & F_{\alpha_1\lambda}-\dfrac{G_{x\lambda}}{G_{xx}}F_{\alpha_1 x} \\ F_{\alpha_2} & F_{\alpha_2\lambda}-\dfrac{G_{x\lambda}}{G_{xx}}F_{\alpha_2 x} \\ F_{\alpha_3} & F_{\alpha_3\lambda}-\dfrac{G_{x\lambda}}{G_{xx}}F_{\alpha_3 x} \end{pmatrix}$$

evaluated at $x=\lambda=0$. Then F is a universal unfolding of G.

Note. One may apply Proposition 2.24 to see that if F is a universal unfolding as in (i) then F is contact equivalent as a parameterized family to $x^3+(\alpha_2+\alpha_3\lambda)x+\alpha_1+\lambda^2$, thus solving our second problem for the winged cusp.

Proof. The heart of the proof has already been completed by the computation of $\tilde{T}G$ in (2.9a) and (2.9b). Given a germ $Q(x,\lambda)$ in $\mathscr{E}_{x,\lambda}$ we may write—where $t(x,\lambda)\in \tilde{T}G$—

(2.33a) $$Q(x,\lambda)=\bar{Q}+\bar{Q}_x x+\bar{Q}_\lambda\lambda+\left(\bar{Q}_{x\lambda}-\frac{\bar{G}_{xx\lambda}}{\bar{G}_{xxx}}\bar{Q}_{xx}\right)x\lambda+t(x,\lambda)$$

or

(2.33b) $$Q(x,\lambda)=\bar{Q}+(\bar{Q}_\lambda-A\bar{Q}_x)\lambda+K(Q)\lambda^2+t(x,\lambda),$$

where $A=\bar{G}_{x\lambda}/\bar{G}_{xx}$ and

(2.34) $$K(Q)=\tfrac{1}{2}[\bar{Q}_{xx}A^2-2\bar{Q}_{x\lambda}A-2\bar{Q}_xB+\bar{Q}_{\lambda\lambda}]$$

and

$$B=\frac{\bar{G}_{x\lambda\lambda}}{2\bar{G}_{xx}}-\frac{\bar{G}_{x\lambda}\bar{G}_{xx\lambda}}{\bar{G}_{xx}^2}+\frac{\bar{G}_{x\lambda}^2\bar{G}_{xxx}}{2\bar{G}_{xx}^3}.$$

In case (i) the proposition follows from Corollary 2.31 directly along with the observation that (2.8a) implies that $\bar{G}_\lambda=\bar{G}_{\lambda x}=0$.

In case (ii) Corollary 2.31 implies that F is a universal unfolding of G if

$$\operatorname{rank}\begin{pmatrix} F_{\alpha_1} & F_{\alpha_1\lambda}-AF_{\alpha_1x} & K(F_{\alpha_1})\\ F_{\alpha_2} & F_{\alpha_2\lambda}-AF_{\alpha_2x} & K(F_{\alpha_2})\\ F_{\alpha_3} & F_{\alpha_3\lambda}-AF_{\alpha_3x} & K(F_{\alpha_3})\\ G_\lambda & G_{\lambda\lambda}-AG_{\lambda_x} & K(G_\lambda)\end{pmatrix}=3.$$

One computes—using (2.18)—that $K(G_\lambda)=\overline{(d^3G)}(v,v,v)\neq 0$ by (2.8b). Also by (2.8b) $\bar{G}_\lambda=0$ and $\bar{G}_{\lambda\lambda}-A\bar{G}_{\lambda x}=\det(\overline{d^2G})/\bar{G}_{xx}=0$. So the proposition is proved.

We are now ready to discuss the problem of classifying—up to contact equivalence—the types of bifurcations which occur in the universal unfolding of a given problem. Suppose one has a bifurcation problem $G(x,\lambda)$ and an l-parameter universal unfolding $F(x,\lambda,\alpha)$, how does one classify in a qualitative way the types of bifurcation diagrams $F(\cdot,\cdot,\alpha)=0$ for various α? A good start at the answer is given by the following theorem. First observe that if G has a universal unfolding then it is contact equivalent to a polynomial and if G is a polynomial then F may also be assumed to be a polynomial. (This is Corollary 2.9 of [4].) Next define

$$(\mathscr{B})=\{\alpha\in\mathbb{R}^l\mid\exists x,\lambda \text{ with } F=F_x=F_\lambda=0 \text{ at } (x,\lambda,\alpha)\},$$

$$(\mathscr{H})=\{\alpha\in\mathbb{R}^l\mid\exists x,\lambda \text{ with } F=F_x=F_{xx}=0 \text{ at } (x,\lambda,\alpha)\},$$

$$(\mathscr{DL})=\{\alpha\in\mathbb{R}^l\mid\exists (x_1,\lambda_1) \text{ and } (x_2,\lambda_2) \text{ with } F=F_x=0 \text{ at both } (x_1,\lambda_1,\alpha) \text{ and } (x_2,\lambda_2,\alpha)\}.$$

These are called the *bifurcation*, *hysteresis*, and *double limit* varieties, respectively.

THEOREM 2.35. *Let $\Sigma=(\mathscr{B})\cup(\mathscr{H})\cup(\mathscr{DL})\subset\mathbb{R}^l$. (Note that Σ is a codimension one algebraic variety in $\mathbb{R}^l$.) Then there exist open neighborhoods $\mathscr{U}$ of 0 in $\mathbb{R}\times\mathbb{R}$ and $\mathscr{V}$ of 0 in $\mathbb{R}^l$ such that if α_1 and α_2 are in the same connected component of $\mathscr{V}\sim\Sigma$ then $F(\cdot,\cdot,\alpha_1)$ and $F(\cdot,\cdot,\alpha_2)$ are contact equivalent on $\mathscr{U}$.*

Proof. This is Corollary 2.16 of [4].

Using this theorem we analyze the local nature of bifurcation diagrams near the winged cusp.

PROPOSITION 2.36. *Let $F(x,\lambda,\alpha)=x^3+(\alpha_2+\alpha_3\lambda)x+\alpha_1+\lambda^2$. Then*

$$(\mathscr{H})=\{\alpha_2^2+\alpha_1\alpha_3^2=0;\ \alpha_2\leqq 0\},\qquad (\mathscr{DL})=\varnothing$$

and $(\mathscr{B})$ *is parameterized by the equations*

$$\alpha_1 = 2x^3 - \frac{\alpha_3^2 x^2}{4}, \qquad \alpha_2 = -3x^2 + \frac{\alpha_3^2 x}{2}.$$

Proof. A short computation.

To visualize how the varieties $(\mathscr{B})$ and $(\mathscr{H})$ intertwine it is perhaps easiest to graph $(\mathscr{B})$ and $(\mathscr{H})$ for α_3 fixed. The results are given in Fig. 2.1. The numbered regions correspond to connected components of the complement of Σ. The lettered regions correspond to various branches of the variety Σ. The bifurcation diagrams are given in Fig. 2.2. (Note that the diagrams associated with Σ are obtained by continuity as one crosses Σ.) Also observe that $(\mathscr{H})$ is just the "Whitney Umbrella" while $(\mathscr{B})$ is a cylinder over a cusp curve. They are pictured in Fig. 2.3.

In the Introduction we stated that the winged cusp is an "organizing center" for bifurcation diagrams associated with the stirred tank reactor described in § 1. We are now in a position to make that statement more precise.

PROPOSITION 2.37. *Let* $G(x, \lambda)$ *be defined on* Ω *in* $\mathbb{R}^2$. *Assume that the following sets of equations are never satisfied in* Ω

(i) $G_{\lambda\lambda} = 0$;

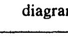
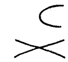
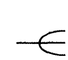
(ii) $G = G_x = G_{xx} = G_{xxx} = 0$; *and*

(iii) $G = G_x = G_\lambda = \det(d^2G) = d^3G(v, v, v) = 0$;

where $(d^2G)(v, v) = 0$. *Then at any point* (x_0, λ_0) *in* Ω *for which* $G(x_0, \lambda_0) = 0$, *the local nature of the bifurcation diagram* $\{G = 0\}$ *is described by one of the eight singularities in Table* 2.1. *Moreover each of these local situations occurs in the universal unfolding of the winged cusp.*

Proof. A simple check shows that conditions (1)–(8) of Table 2.1 yield an exhaustive list for the possibilities for G satisfying (i)–(iii). The normal forms for the singularities (1)–(4) and (6)–(7) are given by Proposition 4.1 of [4]. Singularities (5) and (8) were given in Proposition 2.7.

TABLE 2.1

Defining conditions at (x_0, λ_0)	Normal form	Bifurcation diagram	Codimension
(1) $G = 0$, $G_x \neq 0$	x		0
(2) $G = G_x = 0$, $G_{xx} \cdot G_\lambda \neq 0$	$x^2 \pm \lambda$		0
(3) $G = G_x = G_\lambda = 0$, $G_{xx} \cdot \det d^2G \neq 0$ index $d^2G = 1$	$x^2 - \lambda^2$		1
(4) $G = G_x = G_\lambda = 0$, $G_{xx} \cdot \det(d^2G) \neq 0$ index $d^2G = 0, 2$	$x^2 + \lambda^2$		1
(5) $G = G_x = G_\lambda = \det(d^2G) = 0$ $G_{xx} \cdot (d^3G)(v, v, v) \neq 0$	$x^2 + \lambda^3$		2
(6) $G = G_x = G_{xx} = 0$ $G_{xxx} \cdot G_\lambda \neq 0$	$x^3 \pm \lambda$		1
(7) $G = G_x = G_{xx} = G_\lambda = 0$ $G_{xxx} \cdot G_{\lambda x} \neq 0$	$x^3 \pm \lambda x$		2
(8) $G = G_x = G_{xx} = G_\lambda = G_{\lambda x} = 0$ $G_{xxx} \cdot G_{\lambda\lambda} \neq 0$	$x^3 \pm \lambda^2$		3

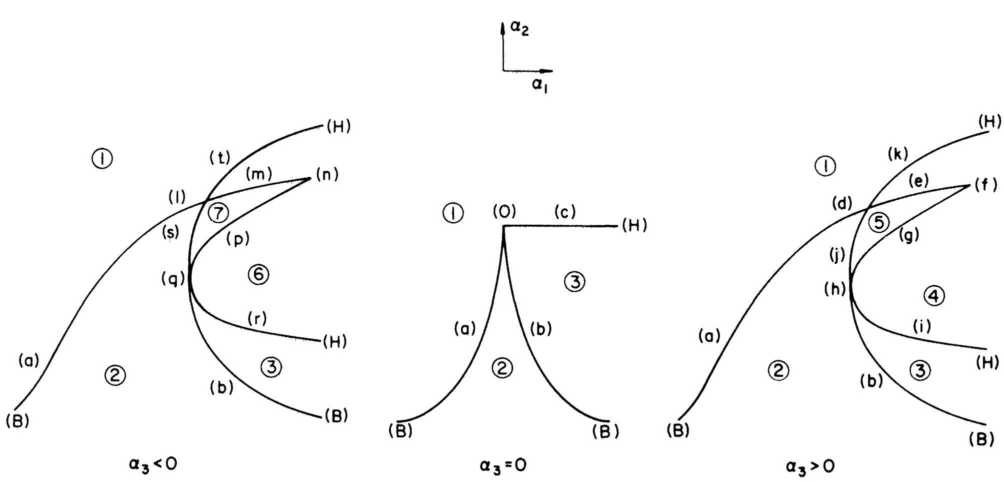
We shall use the following specialized result in our analysis for the stirred tank reactor in the next section.

PROPOSITION 2.38. *Let* $F(x, \lambda, \alpha_1, \alpha_2, \alpha_3) = \alpha_1 + \tilde{F}(x, \lambda, \alpha_2, \alpha_3)$ *be an unfolding of* $G(x, \lambda)$ *as in Proposition* 2.37. *Then* F *is a universal unfolding of* G *if—in each of the eight cases listed in Table* 2.1*—the following conditions are satisfied.*

TABLE 2.2

Case	Condition
(1)–(4)	Always
(5)	$F_{\alpha_3 x}F_{\alpha_2\lambda}-F_{\alpha_2 x}F_{\alpha_3\lambda}\neq 0$
(6)	$\operatorname{rank}\,(F_{\alpha_2 x}\quad F_{\alpha_3 x}\quad G_{x\lambda})=1$
(7)	$\operatorname{rank}\begin{pmatrix} F_{\alpha_2 x} & F_{\alpha_2 xx}-F_{\alpha_2\lambda}\dfrac{G_{xxx}}{G_{x\lambda}} \\ F_{\alpha_3 x} & F_{\alpha_3 xx}-F_{\alpha_3\lambda}\dfrac{G_{xxx}}{G_{x\lambda}} \\ G_{\lambda x} & G_{\lambda xx}-G_{\lambda\lambda}\dfrac{G_{xxx}}{G_{x\lambda}} \end{pmatrix}=2$
(8)	$\operatorname{rank}\begin{pmatrix} F_{\alpha_2 x} & F_{\alpha_2\lambda} & F_{\alpha_2 x\lambda}-\dfrac{G_{xx\lambda}}{G_{xxx}}F_{\alpha_2 xx} \\ F_{\alpha_3 x} & F_{\alpha_3\lambda} & F_{\alpha_3 x\lambda}-\dfrac{G_{xx\lambda}}{G_{xxx}}F_{\alpha_3 xx} \\ 0 & G_{\lambda\lambda} & G_{x\lambda\lambda}-\dfrac{G_{xx\lambda}^2}{G_{xxx}} \end{pmatrix}=3$

Proof. Cases (5) and (8) are easy consequences of Proposition 2.32. The remaining cases are proved in a fashion similar to that proposition.



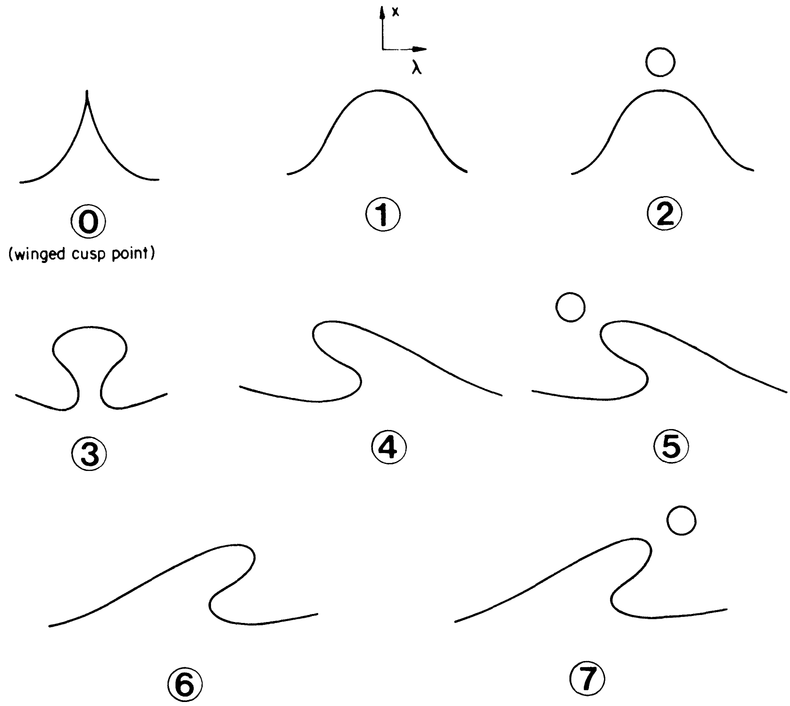
NUMBERS REFER TO OPEN REGIONS
LETTERS REFER TO COMPONENTS OF THE (B) U (H) VARIETY

FIG. 2.1

3. The local nature of the bifurcation diagrams. In § 1 we showed that the steady state solutions to our model chemical reactor are described by the equation:

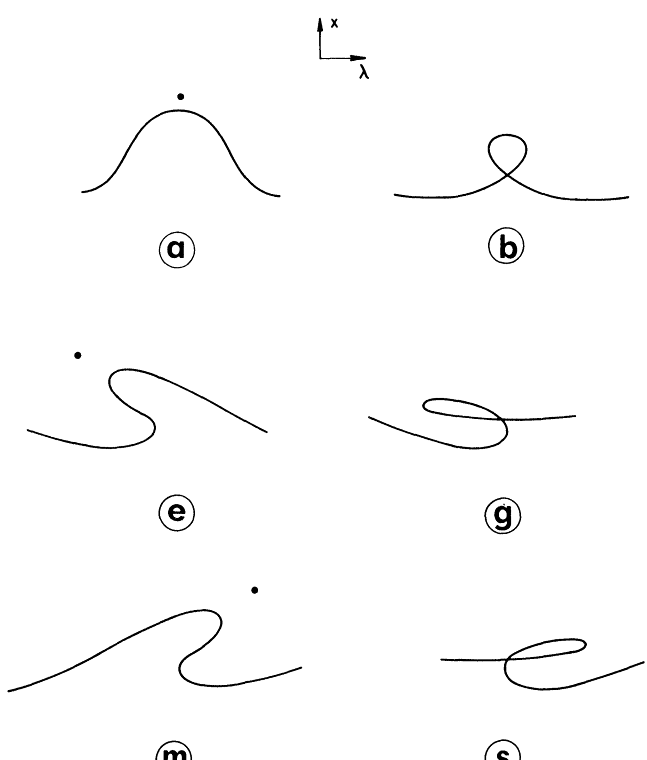
$$G(y,\varepsilon,B,\delta,\eta)=\eta-(1+\varepsilon)y+\frac{B\varepsilon}{1+\varepsilon\delta\mathcal{A}(y)}=0, \tag{3.1}$$

where y is a nondimensionalized temperature, ε is a nondimensionalized flow rate, B, δ and η are parameters, and $\mathcal{A}$ is a reaction rate term which is usually assumed to have the



THE OPEN REGIONS

Fig. 2.2a



OPEN REGIONS ON BIFURCATION VARIETY

Fig. 2.2b

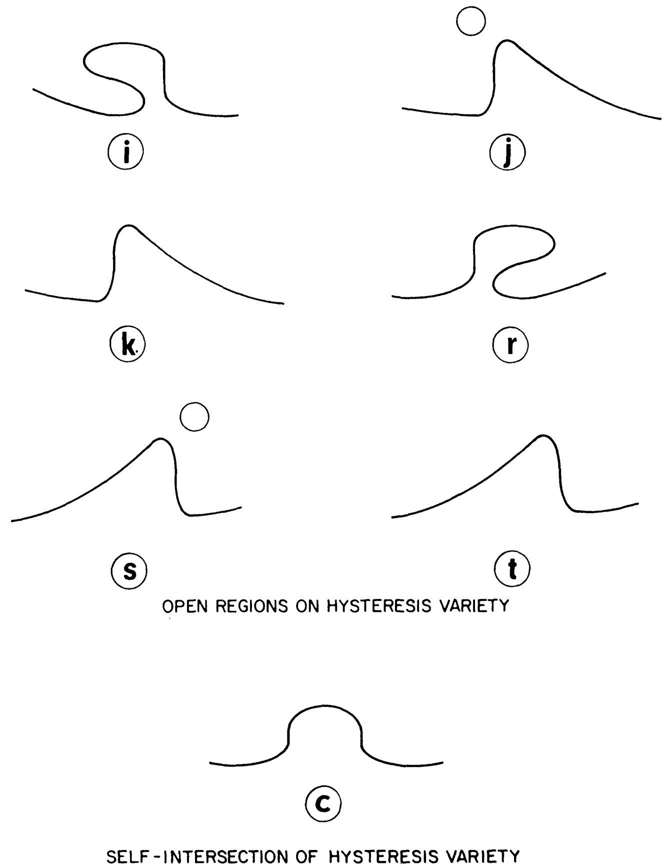


FIG. 2.2c

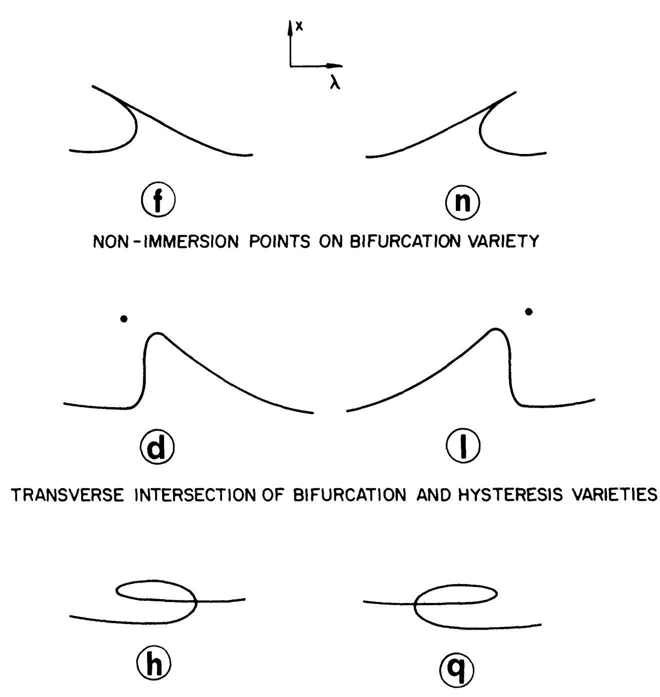
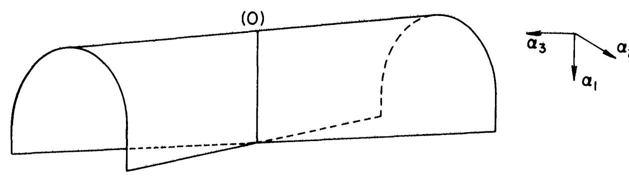
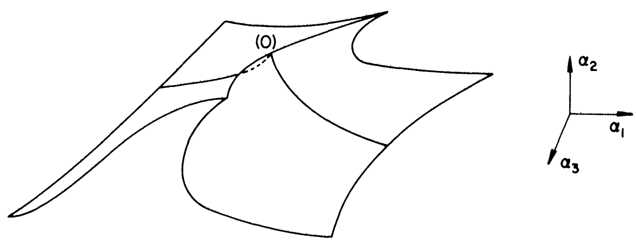


FIG. 2.2d



THE HYSTERESIS VARIETY



THE BIFURCATION VARIETY

FIG. 2.3

form

$$\mathscr{A}(y) = \exp\left(\frac{-\gamma y}{1+y}\right). \tag{3.2}$$

When $\mathscr{A}$ has the form (3.2) we call $\mathscr{A}$ an *Arrhenius term* with activation energy $\gamma > 0$.

The problem we address in this section is the global classification of the local bifurcation problems which appear in this model. We shall prove that for each member of a class of reaction terms which are both open and include the Arrhenius terms when $\gamma > 8/3$, there is a unique winged cusp point and that globally the only local bifurcation problems which occur are those found in the universal unfolding for the winged cusp. Moreover, the physically motivated parameters B, δ, and η turn out to be universal unfolding parameters; it is indeed a curious fact that these parameters—given physically—are the minimum number necessary to determine the qualitative classification. This fact suggests strongly that the winged cusp should be considered as the "organizing center" for this model.

The region in space which we consider is

$$\Omega = \{B > 0, \delta > 0, \eta > -1, y > -1, \varepsilon > 0\}. \tag{3.3}$$

The main assumptions about $\mathscr{A}$ are

$$(3.4)\quad \begin{array}{lll} \text{(A)} & \mathscr{A}(y) > 0, & y > -1, \\ \text{(B)} & \mathscr{A}'(y) < 0, & y > -1, \\ \text{(C)} & \mathscr{A}''(y) > 0, & y > -1, \\ \text{(D)} & \{y, \mathscr{A}\} \equiv \dfrac{2\mathscr{A}'\mathscr{A}''' - 3(\mathscr{A}'')^2}{(\mathscr{A}')^2} < 0, & y > -1. \end{array}$$

The expression $\{y, \mathscr{A}\}$ is called the *Schwarzian derivative* of $\mathscr{A}$ and has been useful in projective geometry. (See E. Cartan [2].) We mention one fact; namely $\{y, g\}=0$ if g is a fractional linear transformation; that is, $g(y)=(ay+b)/(cy+d)$.

A calculation shows that for (3.2) with $y>-1$

(a) $$\mathscr{A}>0,$$

(b) $$\mathscr{A}'(y)=\frac{-\gamma}{(1+y)^2}\mathscr{A}(y)<0,$$

(c) $$\mathscr{A}''(y)=\frac{\gamma+2+2y}{(1+y)^4}\mathscr{A}(y)>0,$$

(d) $$\{y, \mathscr{A}\}=\frac{-\gamma^2}{(1+y)^4}<0.$$

So the assumptions (A–D) are indeed satisfied for the usual Arrhenius terms.

Remark 3.5. Equation (d) shows that $\{y, \mathscr{A}\}=-(\mathscr{A}'/\mathscr{A})^2$. We claim that this differential equation along with the boundary conditions $\mathscr{A}(0)=1$ and $\mathscr{A}(-1)=+\infty$ uniquely define the Arrhenius terms up to γ. For assume $\mathscr{A}=e^g$ then a computation yields $\{y, \mathscr{A}\}=-(g')^2+\{y, g\}$. As $\mathscr{A}'/\mathscr{A}=g'$ we see that $\{y, g\}=0$. As noted above this implies that g is fractional linear; the boundary conditions yield the claim.

Before stating our main results we need two lemmas.

LEMMA 3.6. *Let $\mathscr{A}$ satisfy* (B), (C), *and* (D). *Then there exists a unique point $y_0>0$ such that $\nu=y\mathscr{A}''+\mathscr{A}'=0$.*

Proof. Observe that solutions to $\nu=0$ are obtained as intersections of the two functions $f(y)=-y$ and $g(y)=y+2\mathscr{A}'/\mathscr{A}''$. Assumption (D) shows that g is monotone increasing while f is clearly monotone decreasing to $-\infty$. As $f(0)=0$ and $g(0)=2\mathscr{A}(0)/\mathscr{A}''(0)<0$ the result is proved.

Remark 3.7. For (3.2) $y_0=\sqrt{1+(\gamma^2/4)}-(\gamma/2)$.

LEMMA 3.8. *Let $\mathscr{A}$ satisfy* (A–D). *Then there is at most one point y_z such that $(\mathscr{A}^{-1})''=0$.*

Proof. Let $\mathscr{F}=2(\mathscr{A}')^2-\mathscr{A}\mathscr{A}''$, then $(\mathscr{A}^{-1})''=\mathscr{F}/\mathscr{A}^3$ and we need only find points where $\mathscr{F}=0$. Consider the following identity:

$$2\mathscr{F}'=-\mathscr{A}'\mathscr{A}\{y, \mathscr{A}\}+3\mathscr{A}''\mathscr{F}/\mathscr{A}' \tag{3.9}$$

and observe that if $\mathscr{F}\geqq 0$, then $\mathscr{F}'<0$. This proves the lemma.

Note. If $\mathscr{F}>0$ for all y, let $y_z=+\infty$ and if $\mathscr{F}<0$ for all y, let $y_z=-1$.

Remark. For (3.2), $y_z=(\gamma/2)-1$.

The following list of derivatives of (3.1) will be needed for subsequent computations.

LEMMA 3.10. *Let $\Delta=1+\varepsilon\delta\mathscr{A}(y)$. Then*

(i) $$G=\eta-(1+\varepsilon)y+\frac{B\varepsilon}{\Delta};$$

(ii) $$G_\varepsilon=-y+B/\Delta^2;$$

(iii) $$G_y=-(1+\varepsilon)-B\varepsilon^2\delta\mathscr{A}'/\Delta^2;$$

(iv) $$G_{\varepsilon\varepsilon}=-2B\delta\mathscr{A}/\Delta^3;$$

(v) $$G_{y\varepsilon}=-1-2B\varepsilon\delta\mathscr{A}'/\Delta^3;$$

(vi) $$G_{yy}=B\varepsilon^2\delta Q/\Delta^3 \text{ where } Q=2\varepsilon\delta(\mathscr{A}')^2-\Delta\mathscr{A}'';$$

and

(vii) $$G_{yyy}|_{Q=0} = B\varepsilon^2\delta(3\varepsilon\delta\mathscr{A}'\mathscr{A}'' - \Delta\mathscr{A}''')/\Delta^3.$$

PROPOSITION 3.11. *There exists at most one point* $(y_0, \varepsilon_0, B_0, \delta_0, \eta_0) \in \Omega$ *where the bifurcation problem* $G(y, \varepsilon, B_0, \delta_0, \eta_0) = 0$ *is contact equivalent to the winged cusp on a neighborhood of* (y_0, ε_0).

Moreover if the following assumptions are made on $\mathscr{A}$ *then such a point actually exists in* Ω.

(E) $$(\ln \mathscr{A})''(y_0) > 0,$$

(F) $$y_z > y_0, \quad \textit{i.e.}, \ \mathscr{F}(y_0) > 0 \quad (\textit{Lemma } 3.8),$$

(G) $$y_0^2 + y_0 + \mathscr{A}(y_0)/\mathscr{A}'(y_0) < 0.$$

In fact, these points may be computed as follows:

(i) y_0 *as in Lemma* 3.6,

(ii) $$\varepsilon_0 = -\left.\frac{\mathscr{A} + 2y\mathscr{A}'}{\mathscr{A} + y\mathscr{A}'}\right|_{y=y_0},$$

(iii) $$\eta_0 = -y_0(1+\varepsilon_0),$$

(iv) $$\delta_0 = \left.\frac{-1}{(\mathscr{A} + 2y\mathscr{A}')\varepsilon_0}\right|_{y=y_0},$$

(v) $$B_0 = y_0\Delta_0^2.$$

REMARK 3.12. Assumptions (E) and (G) are satisfied for all Arrhenius terms while (F) is satisfied when $\gamma > 8/3$. As one is really interested in γ large—say of the order of 10—this is a reasonable hypothesis.

Proof. Proposition 2.7 states that to prove this proposition one must show that there is a unique choice of $\beta_0, \delta_0, \eta_0$ yielding a unique solution (y_0, ε_0) to the equation (2.8a) with G, y, ε replacing H, x, λ. Observe that the equations $G_{yy} = G_{y\varepsilon} = 0$ imply that

(3.13a) $$w(2(\mathscr{A}')^2 - \mathscr{A}\mathscr{A}'') = \mathscr{A}'',$$

(3.13b) $$w(\mathscr{A} + 2y\mathscr{A}') = -1,$$

where $w = \varepsilon\delta$. (Here one substitutes $B = y\Delta^2$ into $G_{y\varepsilon}$.) Thus $\mathscr{A}''(b) + (a)$ implies

(3.14) $$2w\mathscr{A}'(\mathscr{A}' + y\mathscr{A}'') = 0.$$

As $w\mathscr{A}' \neq 0$ in Ω we have that y_0 is given by Lemma 3.6. Next solve (3.13a) for

(3.15) $$w = \mathscr{A}''/(2(\mathscr{A}')^2 - \mathscr{A}\mathscr{A}'') = \mathscr{A}''/F.$$

Hence $w_0 = \varepsilon_0\delta_0 > 0$ by (C) and (F). Next substitute $B = y\Delta^2$ into $G_y = 0$ to obtain

(3.16) $$\varepsilon_0 = -1/(1 + y_0 w_0 \mathscr{A}'(y_0)) = -\left.\frac{\mathscr{A} + 2y\mathscr{A}'}{\mathscr{A} + y\mathscr{A}'}\right|_{y=y_0}.$$

The last equality is obtained by solving (3.13b) for w_0. Recall that at y_0, $\mathscr{A}'' = -\mathscr{A}'/y_0$. Thus (E) implies that $\mathscr{A}(y_0) + y_0\mathscr{A}'(y_0) > 0$ and (F) (or (3.13b)) implies $\mathscr{A}(y_0) + 2y_0\mathscr{A}'(y_0) < 0$. So $\varepsilon_0 > 0$ and $\delta_0 > 0$. Now $B_0 = y_0\Delta_0^2 > 0$ where $\Delta_0 = 1 + w_0\mathscr{A}(y_0)$ and from $G = 0$

(3.17) $$\eta_0 = (1+\varepsilon_0)y_0 - B_0\varepsilon_0/\Delta_0 = -(1+\varepsilon_0)y_0.$$

The last equality is obtained as follows: from $G_{\varepsilon y}=0$ derive $\Delta=-2y\mathscr{A}'$ and from $G_y=0$ derive $\Delta=2(\varepsilon+1)/\varepsilon$. Now use (3.17) and (3.16) to obtain

$$\eta_0=\left.\frac{y^2\mathscr{A}'}{\mathscr{A}+y\mathscr{A}'}\right|_{y=y_0}. \tag{3.18}$$

So $\eta_0>-1$ is equivalent to assumption (G).

To complete the proof of the proposition one shows that $G_{\varepsilon\varepsilon}<0$ and $G_{yyy}<0$ at $(y_0, \varepsilon_0, B_0, \delta_0, \eta_0)$. In fact $G_{\varepsilon\varepsilon}<0$ on Ω by (A) and Lemma 3.10 (iv) and $G_{yyy}<0$ on $\Omega\cap\{G_{yy}=0\}$. To obtain this last fact, note that Lemma 3.10 (vi) and (vii) imply that sign (G_{yyy}) on $\{G_{yy}=0\}$ is just sign $(3\varepsilon\delta\mathscr{A}'\mathscr{A}''-\Delta\mathscr{A}''')$. Now

$$3\varepsilon\delta\mathscr{A}'\mathscr{A}''-\Delta\mathscr{A}'''=-\frac{\varepsilon\delta(\mathscr{A}')^3}{\mathscr{A}''}\{y,\mathscr{A}\}<0 \quad \text{on } G_{yy}=0 \tag{3.19}$$

as $\Delta=2\varepsilon\delta(\mathscr{A}')^2/\mathscr{A}''$ on $G_{yy}=0$.

For the following we need one more assumption.

$$\text{(H)}\qquad \frac{(2y\mathscr{A}'''+3\mathscr{A}'')}{3}+\nu\left[\frac{1+\sqrt{1+8y\nu/\mathscr{A}}}{y}+\frac{2\mathscr{A}'}{\mathscr{A}}\right]>0 \quad \text{on } [y_0, y_z].$$

We shall show in the appendix that this inequality is satisfied for Arrhenius terms with $\gamma>2$. Note that at y_0, $\nu=0$ and the first term of (H) is positive by the Schwarzian condition.

PROPOSITION 3.20. *Under the assumptions* (A)–(H) *the only local bifurcation problems which occur in Ω are those which appear in the universal unfolding for the winged cusp.*

Proof. Proposition 2.37 states that Proposition 3.20 is true if none of the following systems of equations is ever satisfied in Ω.

$$G_{\varepsilon\varepsilon}=0, \tag{3.21}$$

$$G=G_y=G_{yy}=G_{yyy}=0, \tag{3.22}$$

$$G=G_y=G_\varepsilon=\det(d^2G)=d^3G(v,v,v)=0, \tag{3.23}$$

where $v\neq 0$ and $(d^2G)(v,v)=0$.

At the end of the proof of Proposition 3.11 we showed that (3.21) and (3.22) are never satisfied in Ω. To analyze (3.23) we need a preliminary result.

As $G_{\varepsilon\varepsilon}$ is never zero we may solve implicitly $G_\varepsilon(y,\varepsilon)=0$ uniquely for $\varepsilon=\varepsilon(y)$. Let $f(y)=G(y,\varepsilon(y))$.

LEMMA 3.24. *The equations* (3.23) *are equivalent to the following system of equations*:

$$f=f'=f''=f'''=0. \tag{3.25}$$

Proof. Observe that

$$f'(y)=G_y(y,\varepsilon(y)), \tag{3.26a}$$

$$f''=G_{y\varepsilon}\varepsilon'+G_{yy}, \tag{3.26b}$$

$$f'''=G_{y\varepsilon\varepsilon}(\varepsilon')^2+2G_{yy\varepsilon}\varepsilon'+G_{yyy}+G_{y\varepsilon}\varepsilon''. \tag{3.26c}$$

By (a) we have that $f=f'=0$ if $G=G_y=G_\varepsilon=0$. Next differentiate the defining equation $G_\varepsilon=0$ to obtain

$$\varepsilon'=-G_{y\varepsilon}/G_{\varepsilon\varepsilon}. \tag{3.27}$$

Thus $f''=0$ if $\det d^2G=0$. Differentiating $G_\varepsilon=0$ a second time yields

$$\varepsilon''=-(G_{yy\varepsilon}+2G_{y\varepsilon\varepsilon}\varepsilon'+G_{\varepsilon\varepsilon\varepsilon}(\varepsilon')^2)/G_{\varepsilon\varepsilon}. \tag{3.28}$$

Substituting (3.28) and (3.27) into (3.26c) yields

$$f'''=(d^3G)(v,v,v) \tag{3.29}$$

by application of (2.18). This proves the lemma.

Of course one may use Lemma 3.10 (ii) to solve for $\varepsilon(y)$ explicitly, obtaining

$$\varepsilon(y)=(\sqrt{B}-\sqrt{y})/\delta\mathscr{A}\sqrt{y}. \tag{3.30}$$

Thus we may take

$$f(y)=\mathscr{A}G(y,\varepsilon(y))=(\eta-y)\mathscr{A}+(\sqrt{y}-\beta)^2/\delta, \tag{3.31}$$

where $\beta=\sqrt{B}$. Since $\mathscr{A}$ is never zero on Ω we still maintain the equivalence of (3.25) with (3.23).

To complete the proof of Proposition 3.20 we must show that (3.25) is never satisfied on Ω. A computation shows that

$$f'(y)=(\eta-y)\mathscr{A}'-\mathscr{A}+(\sqrt{y}-\beta)/\delta\sqrt{y}, \tag{3.32a}$$

$$f''(y)=(\eta-y)\mathscr{A}''-2\mathscr{A}'+\beta/(2\delta y^{3/2}), \tag{3.32b}$$

$$f'''(y)=(\eta-y)\mathscr{A}'''-3\mathscr{A}''-3\beta/(4\delta y^{5/2}). \tag{3.32c}$$

We use the following notation:

$$\nu=\mathscr{A}'+y\mathscr{A}'',\qquad \tau=3\mathscr{A}''+2y\mathscr{A}''',\qquad \mathscr{S}=2\mathscr{A}'\mathscr{A}'''-3(\mathscr{A}'')^2; \tag{3.33}$$

and make the following observations at a solution to (3.25):

$$\eta-y<0, \tag{3.34a}$$

$$\eta-y=6\nu/\tau, \tag{3.34b}$$

$$\beta/\delta=4\mathscr{S}y^{5/2}/\tau, \tag{3.34c}$$

$$\tau<0, \tag{3.34d}$$

$$\nu>0, \tag{3.34e}$$

$$\frac{1}{\delta}=\mathscr{A}-6\nu\mathscr{A}'/\tau+4y^2\mathscr{S}/\tau. \tag{3.34f}$$

It is clear from (3.31) that to solve $f=0$ implies (3.34a). Equations (3.34b) and (3.34c) are obtained from (3.32b) and (3.32c). So (3.34d) follows from (3.34c) as $\beta/\delta>0$ and $\mathscr{S}<0$. Now (3.34e) follows from (3.34b). Finally (3.34f) is obtained from (3.32a).

Substitution of this data into (3.31) yields

$$(\mathscr{A}\tau-6\nu\mathscr{A}'+4y^2\mathscr{S})6\nu\mathscr{A}+y(\tau\mathscr{A}-6\nu\mathscr{A}')^2=0, \tag{3.35}$$

which is an equation in y alone. Letting

$$w=\tau/6\nu \tag{3.36}$$

we obtain from (3.35), noting that $y\mathscr{S}=\mathscr{A}'\tau-3\mathscr{A}''\nu$,

$$\left(w+\frac{\mathscr{A}'}{\mathscr{A}}\right)^2+\frac{1}{y}\left(w+\frac{\mathscr{A}'}{\mathscr{A}}\right)-\frac{2\nu}{y\mathscr{A}}=0. \tag{3.37}$$

As $w<0$ (by (3.34a) and (3.34b)), $\mathcal{A}'/\mathcal{A}<0$ by (A) and (B) and $\nu>0$ (by (3.34e)) we have

$$w=-(1+\sqrt{1+8y\nu/\mathcal{A}})/2y-\mathcal{A}'/\mathcal{A}. \tag{3.38}$$

Hence

$$\tau/3+\nu\left[\frac{(1+\sqrt{1+8y\nu/\mathcal{A}})}{y}+\frac{2\mathcal{A}'}{\mathcal{A}}\right]=0. \tag{3.39}$$

Let y_f be a solution to (3.39) satisfying (3.34). In particular $\nu(y_f)>0$ implies by Lemma 3.6 that $y_f>y_0$. For y_f to generate a solution to (3.25) in Ω it must also satisfy

$$0<\varepsilon(y_f). \tag{3.40}$$

We claim that (3.40) implies that $y_f<y_z$ thus proving the proposition. In particular (3.30) and (3.40) together imply that $\beta>\sqrt{y}$. Using (3.34c) and (3.34f) one obtains

$$1+\frac{\tau\mathcal{A}-6\nu\mathcal{A}'}{4\mathcal{S}y^2}<1, \tag{3.41}$$

which holds only if

$$\tau\mathcal{A}-6\nu\mathcal{A}'>0 \tag{3.42}$$

as $\mathcal{S}<0$. Upon expanding τ we obtain

$$-\tfrac{2}{3}y\mathcal{A}'''<\mathcal{A}''-2\nu\mathcal{A}'/\mathcal{A}. \tag{3.43}$$

Substituting this inequality in (3.39) implies

$$\sqrt{1+8y\nu/\mathcal{A}}<-\frac{\mathcal{A}+4y\mathcal{A}'}{\mathcal{A}}. \tag{3.44}$$

If $(\mathcal{A}+4y\mathcal{A}')|_{y_f}$ is positive then y_f does not correspond to a solution to (3.35) in Ω. So assume that it is negative and square (3.44) to obtain

$$2(\mathcal{A}')^2-\mathcal{A}\mathcal{A}''|_{y_f}=\mathcal{F}(y_f)>0. \tag{3.45}$$

As $\mathcal{F}(y)<0$ for $y\geqq y_z$ by Lemma 3.8 we have that $y_0<y_f<y_z$.

Then by (H) the proposition is proved.

We now state and prove the main result of this section. In particular this result is satisfied for Arrhenius terms when $\gamma>8/3$.

THEOREM 3.46. *Let*

$$G(y,\varepsilon,B,\delta,\eta)=\eta-(1+\varepsilon)y+B\varepsilon/\Delta,$$

where $\Delta=1+\varepsilon\delta\mathcal{A}$ *and* $\mathcal{A}$ *satisfies the conditions* (A)–(H). *Then there exists a unique winged cusp point in* Ω *and for every* $(y',\varepsilon',B',\delta',\eta')$ *the bifurcation problem* $G(y,\varepsilon,B',\delta',\eta')=0$ *is contact equivalent to a bifurcation problem contained in the universal unfolding of the winged cusp point. Moreover* B, δ, *and* η *form universal unfolding parameters for any such bifurcation problem.*

Proof. The first two statements are the results of Propositions 3.11 and 3.20. The proof of the last statement uses Proposition 2.27. In fact, it is sufficient to show that

(a) $$G_{\delta y}G_{B\varepsilon}-G_{By}G_{\delta\varepsilon}\neq 0 \quad \text{on } \Omega;$$

(b) $$\operatorname{rank}(G_{By}\quad G_{\delta y}\quad G_{y\varepsilon})=1 \quad \text{on } \Omega;$$

(c)
$$\operatorname{rank}\begin{pmatrix} G_{By} & G_{Byy}-G_{B\varepsilon}\dfrac{G_{yyy}}{G_{y\varepsilon}} \\ G_{\delta y} & G_{\delta yy}-G_{\delta\varepsilon}\dfrac{G_{yyy}}{G_{y\varepsilon}} \\ G_{y\varepsilon} & G_{yy\varepsilon}-G_{\varepsilon\varepsilon}\dfrac{G_{yyy}}{G_{y\varepsilon}} \end{pmatrix}=2;$$

at points where $G_y=G_{yy}=0$ and

(d)
$$\det\begin{pmatrix} G_{By} & G_{B\varepsilon} & G_{By\varepsilon}-\dfrac{G_{yy\varepsilon}}{G_{yyy}}G_{Byy} \\ G_{\delta y} & G_{\delta\varepsilon} & G_{\delta y\varepsilon}-\dfrac{G_{yy\varepsilon}}{G_{yyy}}G_{\delta yy} \\ 0 & G_{\varepsilon\varepsilon} & G_{y\varepsilon\varepsilon}-\dfrac{G_{yy\varepsilon}}{G_{yyy}}G_{yy\varepsilon} \end{pmatrix}\neq 0$$

at the winged cusp point.

One calculates:

(3.47)
$$\begin{aligned} &\text{(i)} && G_{By}=-\varepsilon^2\delta\mathscr{A}'/\Delta^2;\\ &\text{(ii)} && G_{B\varepsilon}=1/\Delta^2;\\ &\text{(iii)} && G_{\delta y}=B\varepsilon^2\mathscr{A}'(\varepsilon\delta\mathscr{A}-1)/\Delta^3;\\ &\text{(iv)} && G_{\delta\varepsilon}=-2B\varepsilon\mathscr{A}/\Delta^3. \end{aligned}$$

Thus

(3.48)
$$G_{\delta y}G_{B\varepsilon}-G_{By}G_{\delta\varepsilon}=-B\varepsilon^2\mathscr{A}'/\Delta^4>0.$$

So (a) is satisfied. Since $G_{By}>0$ on Ω by (ii) (b) is also satisfied.

To show that (d) holds observe that if a function $f(\varepsilon,\delta)$ has the form $g(\varepsilon\delta)$ then $\varepsilon f_\varepsilon\equiv\delta f_\delta$ so that $f_\varepsilon/f_\delta=\delta/\varepsilon$. Observe—using Lemma 3.10— that this is the case for G_ε, $G_{y\varepsilon}$, and Q. Also note that $G_{yy\varepsilon}/G_{yy\delta}=Q_\varepsilon/Q_\delta$ when $Q=0$. Thus (d) holds if

(3.49)
$$G_{\delta y}\det\begin{pmatrix} G_{B\varepsilon} & G_{By\varepsilon}-\dfrac{G_{yy\varepsilon}}{G_{yyy}}G_{Byy} \\ G_{\varepsilon\varepsilon} & G_{y\varepsilon\varepsilon}-\dfrac{G^2_{yy\varepsilon}}{G_{yyy}} \end{pmatrix}\neq 0.$$

Recall from (3.13) that

(3.50)
$$\varepsilon\delta\mathscr{A}-1=-2\frac{\mathscr{A}+y\mathscr{A}'}{\mathscr{A}+2y\mathscr{A}'}=2/\varepsilon_0>0$$

at the winged cusp point. Now note that $G_{yy}=0$ when $Q=0$ and that $G_{yyB}=\varepsilon^2\delta Q/\Delta^3=0$. So we need only evaluate

(3.51)
$$\det\begin{pmatrix} G_{B\varepsilon} & G_{By\varepsilon} \\ G_{\varepsilon\varepsilon} & G_{y\varepsilon\varepsilon}-G^2_{yy\varepsilon}/G_{yyy} \end{pmatrix}=-\frac{B\delta}{\Delta^5}\left(\frac{2\mathscr{A}'}{\Delta}+\frac{(\mathscr{A}'')^2}{Q_y}\right)>0$$

since $\mathscr{A}'<0$ by (B) and $Q_y<0$ by (3.19).

To complete the proof of the Theorem we must verify (c). Now note that (c) holds if

$$\det\begin{pmatrix} G_{By} & G_{B\varepsilon} & G_{Byy} \\ G_{\delta y} & G_{\delta\varepsilon} & G_{\delta yy} \\ G_{y\varepsilon} & G_{\varepsilon\varepsilon} & G_{yy\varepsilon} \end{pmatrix} \neq 0. \tag{3.52}$$

This is a sufficient though not necessary condition. Recall that $G_{yy} = B\varepsilon^2\delta Q/\Delta^3$ and that $Q = 0$ iff $G_{yy} = 0$. Hence $G_{yyB} = 0$ when $G_{yy} = 0$. Now using the same observation as in the proof of (d) that Q and G_ε are functions of $\varepsilon\delta$ we see that the rank of

$$\begin{pmatrix} G_{\delta\varepsilon} & G_{yy\delta} \\ G_{\varepsilon\varepsilon} & G_{yy\varepsilon} \end{pmatrix} \text{ is } 1.$$

Thus we need only compute

$$\det\begin{pmatrix} G_{By} & G_{B\varepsilon} & 0 \\ G_{\delta y} & 0 & G_{yy\delta} \\ G_{y\varepsilon} & 0 & G_{yy\varepsilon} \end{pmatrix}. \tag{3.53}$$

Note that $G_{B\varepsilon} = 1/\Delta^2 \neq 0$ so this computation reduced to showing

$$D = \det\begin{pmatrix} G_{y\delta} & G_{yy\delta} \\ G_{y\varepsilon} & G_{yy\varepsilon} \end{pmatrix} \neq 0. \tag{3.54}$$

Now

$$D = \frac{B\varepsilon^2\delta}{\Delta^3}\mathcal{F}\det\begin{pmatrix} G_{y\delta} & \varepsilon \\ G_{y\varepsilon} & \delta \end{pmatrix}, \tag{3.55}$$

where $\mathcal{F} = 2(\mathcal{A}')^2 - \mathcal{A}\mathcal{A}''$. Observe that $Q = \varepsilon\delta\mathcal{F} - \mathcal{A}''$ so that $\mathcal{F} \neq 0$ when $Q = 0$. The problem is reduced to computing

$$\delta G_{y\delta} - \varepsilon G_{y\varepsilon} = \varepsilon + B\varepsilon^2\delta\mathcal{A}'/\Delta^2 = -1. \tag{3.56}$$

This last equality is obtained from $G_y = 0$.

Appendix A. We now sketch a proof of:

PROPOSITION A.1. Condition (H) is satisfied for the Arrhenius terms for all $\gamma > 2$.

To prove this proposition we need to show that (3.39) has no solutions on $[y_0, y_z]$. From the derivation of (3.39) this is equivalent to showing that (3.37) has no solutions on $[y_0, y_z]$ when $\tau < 0$. This is our approach.

Note that if $\mathcal{A} = e^g$ then

$$\frac{\mathcal{A}'}{\mathcal{A}} = g', \quad \frac{\mathcal{A}''}{\mathcal{A}} = (g')^2 + g'' \quad \text{and} \quad \frac{\mathcal{A}'''}{\mathcal{A}} = (g')^3 + 3g'g'' + g'''. \tag{A.2}$$

For the Arrhenius terms $g(y) = -\gamma y/(1+y)$. Thus

$$\begin{aligned} &\frac{\mathcal{A}'}{\mathcal{A}} = \frac{-\gamma}{(1+y)^2}, \qquad \frac{\mathcal{A}''}{\mathcal{A}} = \frac{\gamma}{(1+y)^4}[2y+\gamma+2], \\ &\frac{\mathcal{A}'''}{\mathcal{A}} = \frac{-\gamma}{(1+y)^6}[6y^2 + (12+6\gamma)y + 6 + 6\gamma + \gamma^2]. \end{aligned} \tag{A.3}$$

Recall that $\tau = 3\mathscr{A}'' + 2y\mathscr{A}'''$, so

$$\frac{\tau}{\mathscr{A}} = -\frac{6\gamma}{(1+y)^6}\left[y^3 + (1+\tfrac{3}{2}\gamma)y^2 + \left(\frac{\gamma^2}{3} - \gamma - 1\right)y - \left(\frac{\gamma}{2} + 1\right)\right]. \tag{A.4}$$

Since $\nu = \mathscr{A}' + y\mathscr{A}'' > 0$ on $[y_0, y_z]$ we may compute (3.37) in the form

$$\left(\frac{\tau}{6\mathscr{A}} + \frac{\mathscr{A}'}{\mathscr{A}}\frac{\nu}{\mathscr{A}}\right)\left(y\left(\frac{\tau}{6\mathscr{A}} + \frac{\mathscr{A}'}{\mathscr{A}}\frac{\nu}{\mathscr{A}}\right) + \frac{\nu}{\mathscr{A}}\right) - 2\left(\frac{\nu}{\mathscr{A}}\right)^3. \tag{A.5}$$

Compute

$$\frac{\nu}{\mathscr{A}} = \frac{\gamma}{(1+y)^4}(y^2 + \gamma y - 1). \tag{A.6}$$

Then (A.5) is given by

$$\begin{aligned}\frac{\gamma^2}{(1+y)^{12}}\Big[&-\left(\frac{\gamma}{2}+1\right)y^6 - (\tfrac{11}{12}\gamma^2 + 2\gamma + 2)y^5 - (\tfrac{2}{3}\gamma^3 + \gamma^2 + \tfrac{5}{2}\gamma - 1)y^4 \\ &-\left(\frac{2}{9}\gamma^4 + \frac{\gamma^2}{6} - 4\right)y^3 + (\tfrac{2}{3}\gamma^3 - \gamma^2 + \tfrac{5}{2}\gamma + 1)y^2 - (\tfrac{11}{12}\gamma^2 - 2\gamma + 2)y + \left(\frac{\gamma}{2} - 1\right)\Big]\end{aligned} \tag{A.7}$$

Letting $y = (K/\gamma)$ we now show:

LEMMA A.8. *Expression* (A.7) < 0 *for all* $K > 1.2$.

LEMMA A.9. $\tau > 0$ *for all* $K \leqq 1.2$ *when* $\gamma \geqq 2$.

These two lemmas together prove Proposition A.1. Substituting for y in (A.7) and grouping terms by powers of γ yields:

$$c_1\gamma + c_2 + \frac{c_3}{\gamma} + \frac{c_4}{\gamma^2} + \frac{c_5}{\gamma^3} + \frac{c_6}{\gamma^4} + \frac{c_7}{\gamma^5} + \frac{c_8}{\gamma^6}, \tag{A.10}$$

where

$$\begin{aligned} c_1 &= -\left(\frac{2K^3}{9} - \frac{2K^2}{3} + \frac{11K}{12} - \frac{1}{2}\right), \\ c_2 &= -(K-1)^2, \\ c_3 &= -\left(\frac{2}{3}K^4 + \frac{K^3}{6} - \frac{5K^2}{2} + 2K\right), \\ c_4 &= -(K^4 - K^2), \\ c_5 &= -(\tfrac{11}{12}K^5 + \tfrac{5}{2}K^4 - 4K^3), \\ c_6 &= -(2K^5 - K^4), \\ c_7 &= -\left(\frac{K^6}{2} + 2K^5\right), \\ c_8 &= -K^6. \end{aligned} \tag{A.11}$$

We make the following observations:

$$
\text{(A.12)} \qquad
\begin{aligned}
&c_1<0 \quad \text{for } K>1.2,\\
&c_2<0 \quad \text{for all } K,\\
&c_3<0 \quad \text{for } K>1.2,\\
&c_4<0 \quad \text{for } K>1,\\
&c_5<0 \quad \text{for } K>1.2,\\
&c_6<0 \quad \text{for } K>1/2,\\
&c_7<0 \quad \text{for } K>0,\\
&c_8<0 \quad \text{for all } K.
\end{aligned}
$$

This proves Lemma A.8.

Next we compute $\tau(K/\gamma)$—grouped in powers of K—obtaining

$$
\text{(A.13)} \qquad -\frac{K^3}{\gamma^3}-\left(\frac{1}{\gamma^2}+\frac{3}{2\gamma}\right)K^2-\left(\frac{\gamma}{3}-1-\frac{1}{\gamma}\right)K+\left(\frac{\gamma}{2}+1\right).
$$

Note that for any positive γ (A.13) has at most one positive root by Descartes' rule of signs. Since $\tau(0)>0$ and $\tau<0$ for large K, (A.13) has exactly one positive root. So if we evaluate (A.13) at $K=1.2$ and obtain a positive number then Lemma A.9 is proved. This evaluation yields,

$$
\text{(A.14)} \qquad \frac{1}{\gamma^3}(.1\gamma^4+2.2\gamma^3-.96\gamma^2-1.44\gamma-1.728).
$$

Again by Descartes' rule of signs (A.14) has one positive root. Since (A.14) evaluated at $\gamma=0$ is <0 and at $\gamma=2$ is 10.752, Lemma A.9 is proved and Proposition A.1 follows.

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